

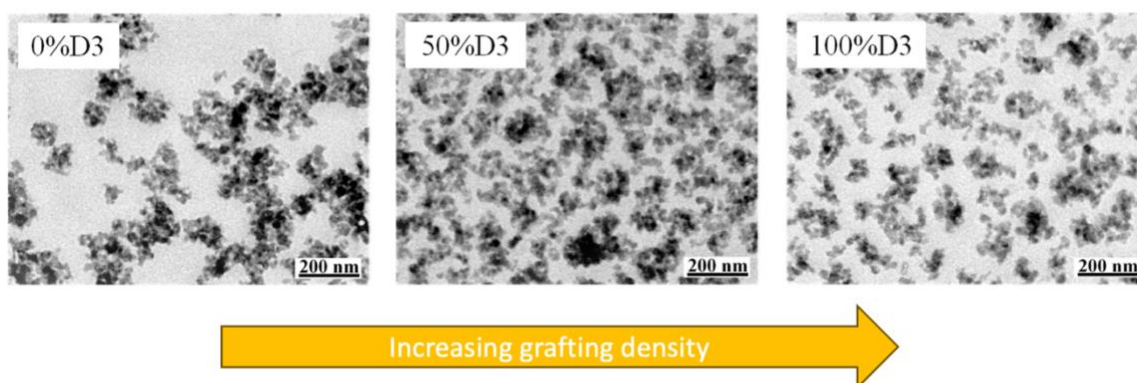
# Effect of Chain Functionalization on the Dynamics of Industrial Polymer-Silica Nanocomposites



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For about 30 years now, silica has been used as the main filler in tread compounds, in partial or total replacement of the more traditional carbon black. Silica has several advantages, but it certainly has a fundamental problem related to its high polarity, which can render it incompatible with the polymers typically used in these compounds. This undesirable effect promotes nanoparticle flocculation, which negatively impacts the mechanical properties of the final product. One way to remedy this issue is to strengthen the filler-matrix interaction through the grafting of polymer chains on the silica surface. Experimental studies of industrial Silica/Styrene-Butadiene rubber (SBR) nanocomposites support this claim and have revealed the emergence of complex filler structures with varying SBR grafting density<sup>1,2</sup>.



Still, the mechanism(s) of filler dispersion through polymer chain functionalization remain a topic of debate. Up to now, most computational studies of polymer nanocomposites have focused on the microscopic aggregation of systems consisting of a few nanoparticles, not allowing for the observation of realistic mesoscale aggregate structures<sup>3,4</sup>. However, modelling the polymeric matrix as an implicit medium can dramatically reduce the computational costs, thus enabling the simulation of a sufficiently large number of nanoparticles<sup>5</sup>. To this end, we plan on developing a Brownian Dynamics computational model that accounts for the attractive interactions between the nanoparticles and the presence of grafted polymer chains, both of which are hypothesized to be the main driving factors of aggregate agglomeration/deagglomeration. Results obtained for various filler volume fractions, interparticle interaction magnitudes & grafting densities will be compared with experimental observations of the mesoscopic structure of industrial Silica/SBR, leading to possible interpretations of the micro-scale mechanisms.

<sup>1</sup> G. Baeza, et al., *Macromolecules*. **46**, 6621 (2013).

<sup>2</sup> G. Baeza, et al., *ACS Macroletters*. **3**, 448 (2014).

<sup>3</sup> V. Sorichetti, et al., *Macromolecules*. **51**, 5375 (2018).

<sup>4</sup> M. Pasquini and G. Raos, et al., *J. Chem. Phys.* **152**, 174902 (2019).

<sup>5</sup> Y. Wang, et al., *Macromolecules*. **52**, 2021 (2019).

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